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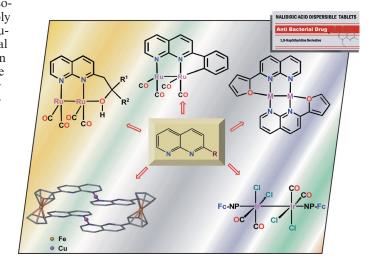




A union formed by chemical societies in Europe (ChemPubSoc Europe) has taken the significant step into the future by merging their traditional journals, to form two leading chemistry journals, the European Journal of Inorganic Chemistry and the European Journal of Organic Chemistry. Three further members of ChemPubSoc Europe (Austria, Czech Republic and Sweden) are Associates of the two journals.

# COVER PICTURE

The cover picture shows various applications of naphthyridine derivatives (NP-R) in dimetal chemistry developed in our laboratory. The cis/trans isomerization of NP-R ligands on a quadruply bonded dimolybdenum(II) platform, axial modulation of the metal-metal bond in dimetal paddlewheel complexes, C-H bond activation and C-C bond formation at the axial site of the [Ru<sub>2</sub>(CO)<sub>4</sub>]<sup>2+</sup> core, the chemistry of ferrocenenaphthyridine hybrid ligands in accessing diiridium compounds and a host of mixed-metal compounds are described in the Microreview by J. K. Bera et al. on p. 4023ff. The multicolour background signifies the versatility of NP-R ligands in dimetal chemistry. The image at the top-right corner emphasizes the importance of naphthyridine derivatives in medicinal chemistry. A line drawing of nalidixic acid, the key ingredient of the anti-bacterial drug GramoNeg (Ranbaxy, India), is seen floating on the image. Contributions from the Design Program, IIT Kanpur and Dr. Nirmal Kumar, principal medical officer at IIT Kanpur, in the preparation of this cover picture are deeply appreciated.



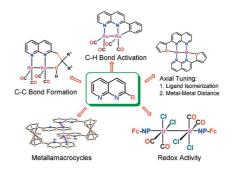
## **MICROREVIEW**

### **Dimetallic Complexes**

J. K. Bera,\* N. Sadhukhan, M. Majumdar ...... 4023-4038

1,8-Naphthyridine Revisited: Applications in Dimetal Chemistry

**Keywords:** Dimetals / Organometallics / Iridium / Self-assembly / N ligands



Recent applications of functionalized naphthyridine ligands (NP-R) in dimetal chemistry are highlighted.

## SHORT COMMUNICATION

### **Uranium Coordination Chemistry**

S. Wu, J. Ling, S. Wang,

S. Skanthakumar, L. Soderholm,

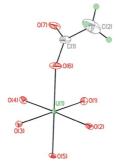
T. E. Albrecht-Schmitt,\* E. V. Alekseev,\*

S. V. Krivovichev,

W. Depmeier ...... 4039-4042

Uranium(VI) Adopts a Tetraoxido Core

**Keywords:** Actinides / Uranium / Oxido ligands / Hydrothermal synthesis / Solidstate reactions / Layered structure / Framework structure / Structure elucidation



The approximately planar tetraoxido core found in Np<sup>VII</sup> and Pu<sup>VII</sup> compounds is unique to the actinides. Here we show that this coordination environment occurs for the ubiquitous element uranium when found in the lower oxidation state of +6.

# **FULL PAPERS**

### **Supramolecular Chemistry**

J. S. Gancheff, R. Q. Albuquerque,

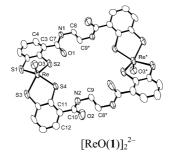
A. Guerrero-Martínez, T. Pape,

L. De Cola, F. E. Hahn\* ...... 4043-4051



A Dinuclear Double-Stranded Oxido Complex of Re<sup>v</sup> with a Bis(benzene-*o*-dithiolato) Ligand

**Keywords:** Oxido complexes / Rhenium(V) / Double-stranded complexes

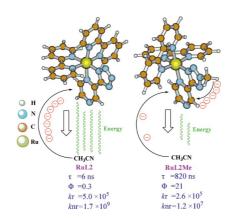


The reaction of [ReOCl<sub>3</sub>(PPh<sub>3</sub>)<sub>2</sub>] with 1,2-bis(2,3-dimercaptobenzamido)ethane (H<sub>4</sub>-1) leads to the formation of a novel double-stranded dinuclear oxido Re<sup>V</sup> complex: [ReO(1)]<sub>2</sub><sup>2-</sup>. DFT calculations were performed to gain insight into the structural and electronic properties of the complex anion.



### **Polarity and Quantum Yields**

The strong polarity of RuL2 is the main reason for a low quantum yield, as it can easily convey energy to the solvent through nonradiative pathways. An electron-donating CH<sub>3</sub> group in RuL2Me can greatly reduce this nonradiative process, which increases its quantum yield.

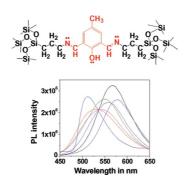


X.-N. Li, Z.-J. Wu, H.-J. Zhang,\* Z.-J. Si, L. Zhou, X.-J. Liu ... 4052–4061

The Reasons for Ligand-Dependent Quantum Yields and Absorption Spectrum of Four Polypyridylruthenium(II) Complexes with a Tetrazolate-Based Ligand: TDDFT Study

**Keywords:** Ruthenium / Absorption / N ligands / Density functional calculations

New supermicroporous luminescent organic-inorganic hybrid microporous material LHMM-1 containing a tunable fluorophore inside the framework has been synthesized in absence of any template and this material shows very strong sensing for metal cations like Fe<sup>3+</sup>, Zn<sup>2+</sup>, Cd<sup>2+</sup> and Hg<sup>2+</sup>.



### **Microporous Tunable Fluorophore**

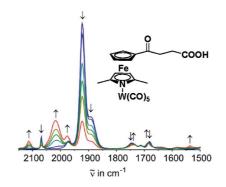
D. Chandra, A. Dutta, A. Bhaumik\* ...... 4062-4068

A New Organic-Inorganic Hybrid Supermicroporous Material Having Luminescence and Ion-Exchange Property

**Keywords:** Sensors / Fluorophore / Fluorescence / Ion exchange / Microporous materials / Organic-inorganic hybrid composites

The synthesis and structure of 2,5-dimethylazferrocene carboxylic acids having IR-active  $W(CO)_5$  markers is reported. Their FTIR spectroelectrochemical studies in OTTLE cell show that IR band shifts of the  $W(CO)_5$  moiety are highly sensitive toward the 2,5-dimethylazaferrocene oxi-

dation state.



### **Tungsten Azaferrocence Complexes**

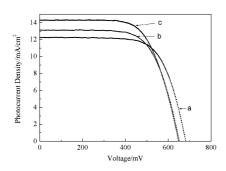
K. Kowalski,\* R. F. Winter, A. Makal, A. Pazio, K. Woźniak ........... 4069–4077

The Synthesis, Structure, and FTIR Spectroelectrochemistry of W(CO)<sub>5</sub> Complexes of 4-Oxo-4-(2,5-dimethylazaferrocen-1'-yl)-butanoic and 5-Oxo-5-(2,5-dimethylazaferrocen-1'-yl)pentanoic Acids

**Keywords:** Metallocenes / Cyclic voltammetry / IR spectroscopy / X-ray diffraction

Titania Nanostructures

Anatase rod-like nanocrystals and nanorings were prepared by a surfactant-free peptization—hydrothermal route, and the resulting TiO<sub>2</sub> has a high adsorption capacity for the ruthenium dye N719.



S. Li, Y. Li, H. Wang,\* W. Fan, Q. Zhang\* ...... 4078–4084

Peptization—Hydrothermal Method as a Surfactant-Free Process toward Nanorod-Like Anatase  ${\rm TiO_2}$  Nanocrystals

**Keywords:** Nanostructures / Hydrothermal synthesis / Sol-gel processes / Crystal growth / Titanium

## **CONTENTS**

### **Molybdenum Complexes**

C. M. Standfest-Hauser, G. Dazinger,

J. Wiedermann, K. Mereiter,

K. Kirchner\* ...... 4085-4093

Molybdenum Carbonyl Complexes Bearing PN Ligands Based on 2-Aminopyridine

**Keywords:** Molybdenum / Carbonyl complexes / Phosphanes / Amines / Oxidative addition / Allyl ligands / Density functional calculations

Mo complexes of the general formula Mo(PN)(CO)<sub>4</sub> containing both achiral and chiral P-N donor bidentate ligands based on 2-aminopyridine were prepared. The oxidative addition of allyl bromide to

Mo(PN)(CO)<sub>4</sub> was studied with PN=N-2-amino-(diisopropylphosphanyl)pyridine (PN-*i*Pr). The mechanism of the oxidative addition was analyzed by DFT/B3LYP calculations.

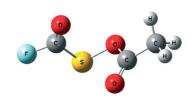
#### **Sulfenic Esters**

M. Cuaquira Reina, C. O. Della Védova, S. E. Ulic,\* H. Willner,

H. Oberhammer ...... 4094-4104

Spectroscopic Characterization and Conformational Properties of S-(Fluoroformyl)-O-(acetyl) Thioperoxide and S-(Fluoroformyl)-O-(trifluoroacetyl) Thioperoxide

**Keywords:** Sulfur / Matrix isolation / Pyrolysis / Vibrational spectroscopy / Conformation analysis / Quantum chemistry



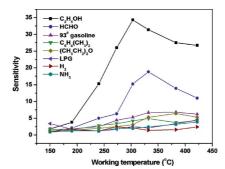
syn-gauche-syn

The conformational properties of sulfenic esters FC(O)SOC(O)CH<sub>3</sub> and FC(O)SOC-(O)CF<sub>3</sub> were studied by vibrational spectroscopy and by theoretical calculations. Both gaseous compounds exhibit conformational equilibria at room temperature; the most stable form possesses *gauche* orientation around the S-O bond and synperiplanar orientation of both carbonyl groups with respect to the S-O bond (*C*<sub>1</sub> symmetry).

## Nanocube Gas Sensors

Simple Solid-State Chemical Synthesis of ZnSnO<sub>3</sub> Nanocubes and Their Application as Gas Sensors

**Keywords:** Oxides / Nanostructures / Solidphase synthesis / Sensors



New ZnSnO<sub>3</sub> nanocubes were synthesized by a simple solid-state chemical reaction between metal salts and NaOH; this process is cheap and proceeds in a relatively simple manner. ZnSnO<sub>3</sub> nanocubes were found to possess good gas-sensing properties for ethanol and methanal; thus these materials may potentially be used as gas sensors.

### **ROP Catalysts**

M. Xue, R. Jiao, Y. Zhang, Y. Yao, Q. Shen\* ...... 4110-4118

Syntheses and Structures of Tris-β-Diketiminate Lanthanide Complexes and Their High Activity for Ring-Opening Polymerization of ε-Caprolactone and L-Lactide

**Keywords:** Synthetic methods / Lanthanides / Lactones / Ring-opening polymerization / Metathesis

Tris- $\beta$ -diketiminate lanthanide complexes and mono- $\beta$ -diketiminate lanthanide dichlorides were synthesized and characterized. The high catalytic activity for the polymerization of  $\epsilon$ -caprolactone and L-lactide shown by tris- $\beta$ -diketiminate lanthanide complexes may be attributed to the activated Ln- $\beta$ -diketiminate bond caused by the steric demand of the three  $\beta$ -diketiminate ligands.



## **Tungsten Hydride Complexes**

Anionic nitrosyl tungsten dihydrides and neutral monohydrides with one or two acidic  $\eta^1$ - or  $\eta^2$ -(2-aminoethyl)dimethylphosphane ligands (edmp) were studied in solution as protonic—hydridic model systems. Complexes of the type W(H)(edmp)(NO)L\_2 (L = phosphane, phosphite) underwent prototropic equilibration with the isomeric  $W(H_2)(NHCH_2CH_2PMe_2)(NO)L_2$  species causing either  $H_2$  release or  $H_W/H_N$  exchange.

Protonic—Hydridic Bifunctionality: The Protonic (2-Aminoethyl)dimethylphosphane Ligand in Nitrosyl Tungsten Hydride Complexes

**Keywords:** Hydride ligands / Structure elucidation / Tungsten / N,P ligands

Optically pure keto- and ester-functionalized C-chiral pyridylarsane ligands were synthesized in high regio- and stereoselectivities via the asymmetric hydrophosphanation reactions using the organopalladium complex containing *ortho*-metalated (*R*)-[1-(dimethylamino)ethyl]naphthalene as the chiral reaction promoter.

 $R = CH_2$ -CO-Ph,  $CO_2CH_3$ 

## **Asymmetric Hydroarsanation**

F. Liu, S. A. Pullarkat, Y. Li, S. Chen, P.-H. Leung\* ...... 4134–4140

Novel Enantioselective Synthesis of Functionalized Pyridylarsanes by a Chiral Palladium Template Promoted Asymmetric Hydroarsanation Reaction

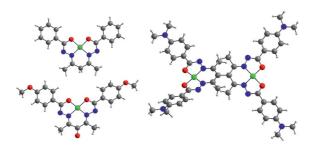
**Keywords:** Asymmetric synthesis / Palladium / As ligands / Template synthesis

# Nickel-Assisted Ligand Transformation

A. Mukhopadhyay, S. Pal\* .... 4141-4148

Nickel-Assisted Oxidative C-C Coupling and Subsequent Cleavage to C=O of Active Methylene Group in a Tetradentate Ligand System: Di- and Mononuclear Complexes with Transformed Ligands

**Keywords:** Nickel / Ligand transformation / C-C coupling / Structure elucidation / EPR spectroscopy / Magnetic properties



Pyrazolines derived from acetylacetone and 4-R-benzoylhydrazine and  $Ni(O_2CCH_3)_2$ · $4H_2O$  in boiling methanol provide  $Ni^{II}$  species, [Ni(H<sup>R</sup>L)], [H<sub>3</sub><sup>R</sup>L = acetylacetone bis(4-R-benzoylhydrazone)] (top left), while

prolonged exposure of the reaction mixture to air provides a formally di-Ni<sup>III</sup> species, [Ni(RL-RL)Ni] (right), which transforms, with H<sub>2</sub>O/O<sub>2</sub>, to a new Ni<sup>II</sup> species, [Ni(RLO)] (bottom left).

Iron(II) complexes (Fe1–Fe7) ligated by 2-(2-benzoxazolyl)-6-[1-(arylimino)ethyl]pyridines showed moderate to good activities (up to ca.  $10^6\,\mathrm{g\,mol^{-1}Fe\,h^{-1}\,bar^{-1}}$ ) toward ethylene oligomerization and polymerization with high selectivity in forming vinyl-terminated oligomers or polyethylene waxes upon activation with modified methylaluminoxane.

**Ethylene Oligomerization** 

2-Benzoxazolyl-6-[1-(arylimino)ethyl]pyridyliron(II) Chlorides as Ethylene Oligomerization Catalysts

**Keywords:** Iron / N ligands / Oligomerization / Polymerization

# **CONTENTS**

### ansa-Tris(allyl) Complexes

S. A. Sulway, R. Girshfeld, S. A. Solomon,

C. A. Muryn, J. Poater, M. Solà,

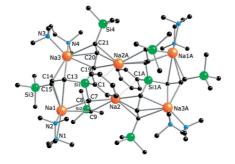
F. M. Bickelhaupt,\*

R. A. Layfield\* ...... 4157-4167



Alkali Metal Complexes of Silyl-Substituted ansa-(Tris)allyl Ligands: Metal-, Co-Ligand- and Substituent-Dependent Stereochemistry

**Keywords:** Allyl ligands / Lithium / Sodium / Potassium / Stereochemistry



The structure and stereochemistries of a series of silyl-substituted *ansa*-tris(allyl) complexes of lithium, sodium and potassium are dependent on the radius of the metal cation, the denticity of the co-ligands and the substituents on the silicon atoms.

Supporting information on the WWW (see article for access details).

If not otherwise indicated in the article, papers in issue 26 were published online on August 31, 2009

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